MODELING FISSION RATES IN MCNPX

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To accurately predict the absolute delayed gamma responses in a neutron interrogation experiment, we need to know the number of fissions produced by irradiation. This quantity depends very heavily on the experimental geometry and the source neutron spectrum. MCNPX makes for a convenient tool to carry out this kind of complex calculation.

Our proposed geometry uses of a 2.5MeV D-D neutron generator, with source strength of 10^8 neutrons per second. This device is surrounded by a large block of polyethylene moderator to thermalize the source neutrons. Appendix A presents 2D projections of this setup.

There was confusion in our initial simulations of the fission probabilities. It was somewhat unclear what units MCNPX used to report the probabilities. We had simply assumed that the output tallies represented the number of fissions per source neutron across the entire tally cell. This turns out to be incorrect—MCNPX also normalizes the results to the tally cell volume, giving fissions per source neutron per cm^3. Our use of the "tally multiplier" option on a cell flux tally multiplied the neutron flux (n/cm^2) by the ^{235}U atom density (atoms/barn·cm) by the reaction cross-section (barns), which gave units of reactions/cm^3.

I have run several test simulations to verify this result. The first directs a monoenergetic beam of thermal (0.025eV) neutrons along the y-axis towards a thin, pure U-235 target. Since the target is thin, the high-energy neutrons produced from fission with likely escape the sample without being absorbed. This allows a direct comparison with an analytic calculation.

Suppose a given reaction has a cross section σ. Let a mono-energetic, mono-directional beam of particles be incident on a thin target of thickness d and atom density N. The number of source particles that pass to the other side of the sample is given by

$$\mathbf{X = X_0 \, e^{-N \sigma d}}$$

where X_0 is the original source strength. Therefore, the number of reactions that occur in the sample is simply

$$\mathbf{R = X_0 - X = X_0 - X_0 \, e^{-N \sigma d} = X_0 \left(1 - e^{-N \sigma d} \right)}$$

We can, of course, get N from the material density ρ, the molar mass M, and Avogadro's number A. That is, $N = \rho * A / M$.

In my test case, I used pure U-235, with a density of 19.1 g/cc and molar mass of 235.044 g/mol. The target thickness is 0.01 cm, and the thermal fission cross-section for U-235 is 580 barns. Plugging these quantities into the above expression for the number of reactions, we get

$$\mathbf{R = 0.247\ X_0}$$

i.e. 24.7% of the incident neutrons react in the thin sample.

The MCNPX tally for this simulation gave a thermal fission factor of 7.82066 per source neutron. This number clearly does not represent fissions per source neutron—there is very little neutron multiplication in the small target. Note, then, that the cylindrical sample has a radius of 1 cm and thickness of 0.01cm, giving a volume of 0.0314159 cc. Multiplying the volume and the fission factor gives $7.82066 \cdot 0.0314159 = 0.2457$, which is very close to the expected reaction probability. (The difference is likely due to the statistical uncertainty from the relatively short MCNPX calculation.)

Appendix B contains the MCNPX input file used for the analytical comparison.

The next series of MCNPX simulations used the full experimental geometry from Appendix A, with a single HEU-pin as a target. (The UO_2 pin is enriched to 43% ^{235}U and has a mass of 1.50777g, a radius of 0.25cm, a length of 0.7cm, and a density of 10.97 g/cm^3.) For these tests, I varied the entry for the "SD" input card, which controls the tally cell volume. According to the MCNPX manual and my own observation, it is required when MCNPX cannot calculate the cell volume automatically. (This occurs for multi-part or a-symmetric cells.) The SD card parameter only affects the tally output, and was the only aspect I changed between simulations.

The neutron flux through the cell was nearly constant for all runs, at 1.34312×10^{-4} neutrons per cm^2 per source neutron. The table below lists the outputs for the different values of SD that I used.

VALUE OF THE "SD"PARAMETER	FISSION FACTOR
SD card missing (default)	5.94656×10^{-5}
0.1374 cm^3 (actual target volume)	5.94850×10^{-5}
0.33 cm^3	2.47674×10^{-5}
1 cm^3	8.17323×10^{-6}
2 cm^3	4.08662×10^{-6}

TABLE: Effects of the SD card on reported fission factors

It is pretty clear that MCNPX divides the fission probability by the cell volume (specified by the SD parameter). The fission probability for SD = 2 cc is twice as low as the one for SD = 1 cc, which in turn is 3 times lower than the one with SD = 0.33 cc. The factors aren't quite integers, but that is due to the low level of statistics accumulated during each run.

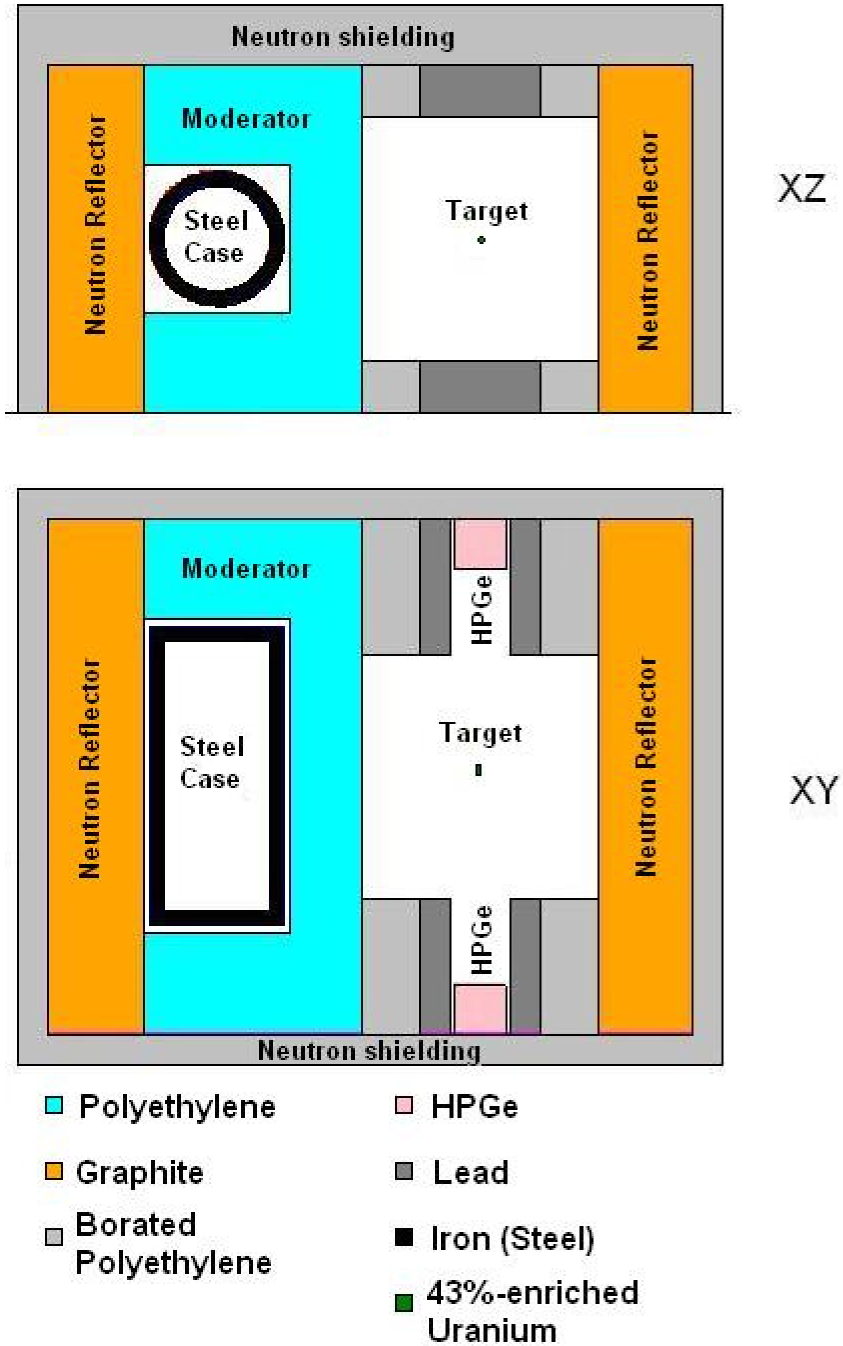
See Appendix C for the MCNPX input used for these tests.

We can conclude that the fission probabilities are indeed output in fissions per cc per source neutron. As a side-note, to find the total fissions in the cell, one could specify the tally volume to be 1 cm^3, i.e. use SD = 1.

In light of the above results, I ran a long, 12-hour simulation for the experimental geometry to gather better statistics. (I used the input deck from Appendix C with a much higher value for the NPS parameter.) As with the tests above, I used a single HEU pellet as a target for simplicity. Taking the volume of the pellet into account, the fission probability is 6.38×10^{-6}, with an uncertainty of 2.15%. An array of 12 such pins, then, should give something on the order of 7.66E-5 fissions per source particle. This is about a factor of 14.4 less than the original number we reported (1.1E-3).

Given a source strength of 10^8 neutrons per second, a 200ms irradiation time should produce 127.6 fissions in a single HEU pellet.

APPENDIX A: EXPERIMENTAL GEOMETRY



APPENDIX B: MCNPX INPUT FOR A SIMPLE ANALYTICAL COMPARISON

```
U-235 Fission Simulation
c Begin Cell Section
1 1 -19.1        -1 2 -3         imp:n=1   $ Uranium cylinder
100 0            #1 -100         imp:n=1   $ Vacuum around sample
999 0            100             imp:n=0   $ Void
c End Cell Section

c Begin Surface Section
1 CY 1
2 PY 1
3 PY 1.01
50 PY 0
100 SO 10
c End Surface Section

c Begin Data Section
c --- Building Materials
m1 92235.66c 1                              $ Pure U-235
F4:n 1
E4 1e-7 1e-6 1e-5 1e-4 1e-3 1e-2 1e-1 1 10 100 1000
F14:n 1
E14 1e-7 1e-6 1e-5 1e-4 1e-3 1e-2 1e-1 1 10 100 1000
FM14 (-1 1 (-6))
SD14 0.0314159
mode:n
sdef pos=0 0 0 erg=2.5E-8 par=n sur=50 vec=0 1 0 dir=1
nps  5e6
print 40 140 150
```

APPENDIX C: MCNPX INPUT FOR THE EXPERIMENTAL GEOMETRY

```
Neutron Generator for U-235/U-238 Fission Detection
c ----- flux/fission rate test: vary only direct moderator 8cm
c --- To vary moderator thickness, change x-vectors for
c --- surfaces 10 and 300, as well as translation #1
c --- This is for a *SINGLE* HEU pin
c Begin Cell Section
1 7 -2.1      -1                imp:n=1   $ Left-most reflector
2 5 -0.97     -10 11            imp:n=1   $ Poly around source
10 6 -0.97    -20 21            imp:n=1   $ Left borated poly
11 4 -11.34   -30 31 32         imp:n=1   $ Pb shield
30 6 -0.97    -50 51            imp:n=1   $ Right borated poly
90 7 -2.1     -60               imp:n=1   $ Right-most reflector
100 2 -0.0012754  (-31:-32) #300 #400 #450 imp:n=1   $ Cavity w/ target
110 2 -0.0012754  #200 #201 #202 -11 imp:n=1   $ Cavity w/ cylinder
200 1 -7.85 100 -101 -104 105    imp:n=1   $ Steel sample cylinder
201 1 -7.85 -101 -102 104        imp:n=1   $ Steel cylinder cap
202 1 -7.85 -101 -105 103        imp:n=1   $ Steel cylinder cap
300 3 -10.97 -200 -211 212       imp:n=1   $ Uranium target
400 8 -5.32 -150 -300 151        imp:n=1   $ Ge detector #1
450 8 -5.32 -150 -300 -152       imp:n=1   $ Ge detector #2
900 2 -0.0012754 300 -301        imp:n=1   $ Air around setup
999 0            301             imp:n=0   $ Void
c End Cell Section

c Begin Surface Section
1 BOX -40.4 -41.4 -31.4   28 0 0   0 82.8 0   0 0 62.8
c --- 10-11 used for poly moderator around source
10 BOX -12.4 -41.4 -31.4   36.8 0 0   0 82.8 0   0 0 62.8
11 BOX -12.4 -26.4 -12.4   24.8 0 0   0 52.8 0   0 0 24.8
c --- 20-21 used for left borated poly
20 1 BOX 0 -41.4 -31.4   9.7 0 0   0 82.8 0   0 0 62.8
21 1 BOX 0 -20.48 -20.48   9.7 0 0   0 40.96 0   0 0 40.96
c --- 30-32 used for Pb detector shielding
30 1 BOX 9.7 -41.4 -31.4   20 0 0   0 82.8 0   0 0 62.8
31 1 BOX 14.7 -41.4 -5   10 0 0   0 82.8 0   0 0 10
32 1 BOX 0 -20.48 -20.48   39.4 0 0   0 40.96 0   0 0 40.96
c --- 50-51 used for right borated poly
50 1 BOX 29.7 -41.4 -31.4   9.7 0 0   0 82.8 0   0 0 62.8
51 1 BOX 29.7 -20.48 -20.48   9.7 0 0   0 40.96 0   0 0 40.96
60 1 BOX 39.4 -41.4 -31.4   31.9 0 0   0 82.8 0   0 0 62.8
c --- 100-105 used for steel capsule
100 CY 10.765
101 CY 11.4
102 PY 25.4
103 PY -25.4
104 PY 24.765
105 PY -24.765
c --- 150-152 used for Ge detectors
150 1 C/Y 19.6 0 4.38
151 1 PY 34.96
152 1 PY -34.96
c --- 200-216 used for the uranium pins
```

```
200 1 C/Y 19.9 0 0.25
211 1 PY 0.35
212 1 PY -0.35
c --- 300-301 used for boundaries
300 BOX -40.4 -41.4 -31.4   136.1 0 0   0 82.8 0   0 0 62.8
301 SO 200
c End Surface Section

c Begin Data Section
c --- Building Materials
m1 26000.55c 1                              $ Natural Fe
m2 7014.66c 0.79 8016.66c 0.21                  $ Air
m3 92235.66c 0.43 92238.66c 0.57 8016.66c 2         $ 43% HEU MOX
m4 82000.50c 1                              $ Natural Pb
m5 12000.66c 0.33  1001.66c 0.67                $ Polyethylene
m6 12000.66c -0.814 1001.66c -0.186 5010 -0.05  $ Borated polyethylene
m7 12000.66c 1                              $ Natural C (Graphite)
m8 32000.67c 1                              $ Natural Ge
c --- Tally Materials
m100 92235.66c 1
m101 92238.66c 1
*TR1 24.4 0 0   0 90 90   90 0 90   90 90 0 $ Translation for right half of
setup
F4:n 300
E4 1e-7 1e-6 1e-5 1e-4 1e-3 1e-2 1e-1 1 10 100 1000
F14:n 300
FM14 (-0.1433 100 (-6))
        (-0.19 101 (19:20))
c SD14 0.1374
mode:n
sdef pos=0 0 0 erg=2.5 par=n
nps  5e5
print 40 140 150
```